Lawrence Livermore National Laboratory

Computation Directorate

Enabling Science and Technology

2003 Annual Report

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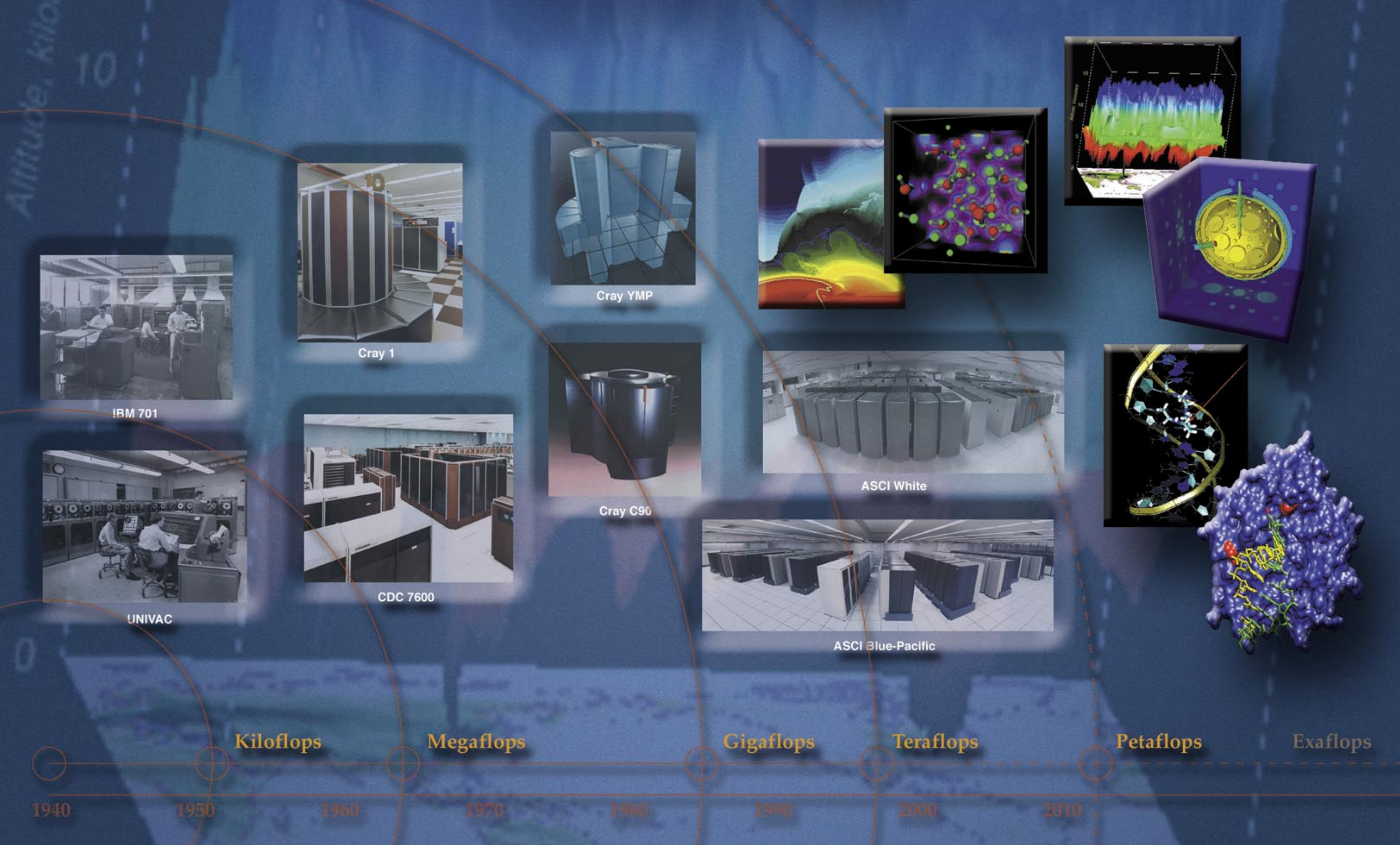
Advances in High-Performance Computing at LLNL



1.00 Computing at Lawrence Livermore in 2003

Dona L. Crawford
Associate Director for Computation

Big computers are icons: symbols of the culture, and of the larger computing infrastructure that exists at Lawrence Livermore. Through the collective effort of Laboratory personnel, they enable scientific discovery and engineering development on an unprecedented scale. For more than three decades, the Computation Directorate has supplied the big computers that enable the science necessary for Laboratory missions and programs.

Livermore supercomputing is uniquely mission driven. The high-fidelity weapon simulation capabilities essential to the Stockpile Stewardship Program compel major advances in weapons codes and science, compute power, and computational infrastructure. Computation's activities align with this vital mission of the Department of Energy.

Increasingly, non-weapons Laboratory programs also rely on computer simulation. World-class achievements have been accomplished by LLNL specialists working in multi-disciplinary research and development teams. In these teams, Computation personnel employ a wide array of skills, from desktop support expertise, to complex applications development, to advanced research.

Computation's skilled professionals make the Directorate the success that it has become. These individuals know the importance of the work they do and the many ways it contributes to Laboratory missions. They make appropriate and timely decisions that move the entire organization forward. They make Computation a leader in helping LLNL achieve its programmatic milestones. I dedicate this inaugural Annual Report to the people of Computation in recognition of their continuing contributions.

I am proud that we perform our work securely and safely. Despite increased cyber attacks on our computing infrastructure from the Internet, advanced cyber security practices ensure that our computing environment remains secure. Through Integrated Safety Management (ISM) and diligent oversight, we address safety issues promptly and aggressively. The safety of our employees, whether at work or at home, is a paramount concern.

Even as the Directorate meets today's supercomputing requirements, we are preparing for the future. We are investigating open-source cluster technology, the basis of our highly successful Mulitprogrammatic Capability Resource (MCR). Several breakthrough discoveries have resulted from MCR calculations coupled with theory and experiment, prompting Laboratory scientists to demand ever-greater capacity and capability. This demand is being met by a new 23-TF system, Thunder, with architecture modeled on MCR.

In preparation for the "after-next" computer, we are researching technology even farther out on the horizon—cell-based computers. Assuming that the funding and the technology hold, we will acquire the cell-based machine BlueGene/L within the next 12 months.

Achievements in 2003

Looking back over 2003, and looking forward to the possibilities of the next few years, I am excited about the ways Computation has enabled broad scientific opportunities and facilitated discovery, and the many ways we will continue to contribute to future LLNL initiatives. A number of achievements in 2003 enabled Laboratory initiatives, programs, and projects. They are briefly described below.

- **Major new computer capabilities augment LLNL's classified and unclassified HPC environment**
  The classified environment added three machines with more than 21-TF peak capability;

the unclassified 23-TF IA64 Thunder cluster began science runs.

- **HPC clusters using open-source systems software become available for production**
  Together with several industrial partners, Computation deployed a new version of the LLNL Linux Software Stack (operating system, parallel file system, and resource management system). Production-quality, large-scale HPC Linux clusters are now a reality. The multi-cluster simulation environment based on a single Lustre File System is impacting every program at LLNL.

- **New algorithms facilitate largest-ever ALE3D simulations**
  Within the nation's Stockpile Stewardship Program, large three-dimensional structural dynamics simulations are now performed on meshes with 610 million degrees of freedom, using 4032 processors of ASCI White. This is 100 times larger than the simulations of only three years ago, with 10 times the number of processors.

- **ICCS software operates in NIF Early Light**
  The NIF Integrated Computer Control System software is more than 75% complete. ICCS is used to commission and operate the first four beams as part of the successful NIF Early Light campaign, demonstrating NIF's end-to-end capability.

- **Bioinformatics efforts expand national biodefense**
  Computation partnered with NAI, BBRP, and Engineering to develop the Biological Aerosol Sentry and Information System (BASIS). This system enables early detection of biological pathogens. Computation researchers also developed a new, parallel algorithm that is ten times faster than the previous version and will enable the processing of genomes of larger organisms.

- **ARGUS integrated security system deploys to LANL**
  ARGUS, DOE's standard high-security system, protects assets at LLNL, Pantex, INEEL, DOE HQ, and now LANL. ARGUS includes personnel access control booths, alarm stations, map-based alarm reporting systems, and a closed circuit TV video assessment system.

- **Security improves through centralized management of usernames and passwords**
  Almost 100 LLNL business applications now authenticate through a single system, providing enhanced security of institutional services. Remote access is available through the One-Time Password (OTP) authentication system.

- **Major cyber vulnerabilities thwarted**
  Through internal collaboration, Windows vulnerabilities were identified and a response process was defined to both combat the vulnerabilities and to alert LLNL programs of the potential threat from malicious computer code. Several government and commercial sites were affected by the malicious-exploit computer code requiring them to disconnect from the Internet, but there were no major infections or operational impacts to the Laboratory.

- **Computation leads Lab-wide SQA efforts**
  Computation spearheaded the development of the institutional Software Quality Assurance (SQA) policy that was recently approved. The policy calls for a multi-tiered, risk-based, tailorable approach to software quality assurance and engineering practices. The Directorate is coordinating the development of an implementation plan.

- **Computation pilots the DHS ASC program**
  Computation is leading the Advanced Scientific Computing (CASC) research program for the Department of Homeland Security (DHS). LLNL organized a national workshop to define program needs and is now building a national program

Recognition and Awards in 2003

In addition to these major accomplishments, it is always gratifying to see Computation personnel and programs recognized by others for their outstanding contributions to the Directorate, the Laboratory, or the profession. A summary of such awards is noted below.

Teller Fellowship Award

Michel G. McCoy and Mark K. Seager received the fourth annual Teller Fellowship Award. Each award allows the recipient to do a year of self-directed work that will benefit the Laboratory. Mike and Mark plan to recruit a computer architect to focus on analyzing technologies that might scale to petaflop-class systems (10^{15} operations per second, peak speed) and beyond. Their goal is to explore cluster and alternative technologies for petaflop-class systems later this decade.

R&D 100 Award

Tom Slezak, Linda Ott, and Mark Wagner received a prestigious R&D 100 Award for their contributions to the BASIS team. BASIS, as described above, permits early detection of biological pathogens, and detectors have been successfully deployed at multiple locations across the country. Livermore team members serve four directorates: Nonproliferation, Arms Control and International Security; Biology and Biotechnology Research Program; Computation; and Engineering. An additional participant came from Los Alamos National Laboratory.

Service to the SC Conference Series

James McGraw chaired SC 2003, the premier conference in high-performance computing and networking. The annual conference, held in Phoenix, AZ, attracted more than 7,600 attendees, making it the largest and most successful in the 15-year history of the series.

Engineering Profession Distinguished Service Award

Linda Dibble accepted the Engineering Profession Distinguished Service Award from the San Joaquin Engineering Council. This award recognized her community outreach activities for the Lab, including the Tri-Valley Science & Engineering Fair and the Pleasanton Partnership in Education, among many others. Additionally, Linda has been a member of the Expanding Your Horizons consortium board, and since 1998 has co-chaired its annual San Joaquin conference, designed to nurture girls' interest in science and math courses, and to encourage them to consider science and math based career options such as engineering, computer science and biometrics.

Data Mining Awards and Recognition

Chandrika Kamath and Erick Cantú-Paz, both of the Sapphire Project, were issued a U.S. patent for a Parallel Object-Oriented Data Mining System.

Figure 1.00-1 The Terascale Simulation Facility will showcase ASCI Purple in 2005.

Erick Cantú-Paz is one of five initial fellows named to the International Society for Genetic and Evolutionary Computation.

Annual Report Overview

This first-ever Computation Directorate Annual Report compiles snapshots of programs and projects across the Directorate. It is divided into sections that explain and describe facets of our work. The following synopsis briefly outlines the report.

Section 2
Providing Desktops to Teraflops Computing

In 1995, at the beginning of the Advanced Simulation and Computing Program (originally the Accelerated Strategic Computing Initiative, or ASCI), we examined the kinds of physical phenomena we would need to simulate, when we would need to generate these simulations, and how quickly we would need calculation results returned. This analysis determined the computers we would acquire through partnerships with industry leaders. Our goal was to obtain, by 2004, a computer system capable of 100 trillion floating-point operations per second (100 TF).

Livermore, Los Alamos, and Sandia, the three national laboratories involved in ASCI, have fielded increasingly powerful massively parallel supercomputers. ASCI Purple, arriving at Livermore mid-2005, will fulfill the original 100-TF goal. But the story does not end there. Successful simulation environments require more than huge computers with maximum peak speeds. They require computing and communications environments integrated from desktops to teraflops, with associated support and services at all levels. They require infrastructure—storage systems, visualization capabilities, networks, compilers, and debuggers—all working together.

Section 3
Developing Applications Software

World-class science on advanced architectures such as ASCI Purple, Thunder, or BlueGene/L also requires the expertise of individuals who can direct advanced applications development. It requires code development, physics modeling, and algorithms improvements; it requires computer applications runs and analysis; it requires computer security compliance and technology integration; and, it requires information technology expertise.

In addition, many projects require personnel who have real-time systems expertise, database management capability, specialized systems management capability, specialized systems knowledge, or specialized backgrounds in a particular area of computer science or mathematics. Regardless of the individual's background or project assignment, the work is undertaken in a balanced and integrated manner using a systems approach.

Section 4
Computing Research and Development

Directorate researchers actively advance the computational technologies that facilitate Laboratory terascale scientific simulation. Our research is broad in scope and consistent in vision. It enables Laboratory scientists to harness massively parallel machines with thousands of processors for predictive simulation of complex physical phenomena.

The Directorate fosters numerous research projects, including scalable numerical algorithms, discretization methodologies, object-oriented and component-based software, multiresolution data management and visualization, and system software. Computation personnel collaborate with programmatic partners to build and then to use these technologies in breakthrough scientific investigations in the defense, environmental, energy, and biological sciences.

Section 5
Additional Information

None of our work is performed in a vacuum. We collaborate often and extensively with almost 80 national laboratories, academic institutions, and industrial partners. We actively seek the innovation, sound judgment, and disciplined execution that lead to the collective success of the Laboratory's mission. Our partners and collaborators are listed in Section 5. Additionally, a cross-reference of acronyms is provided to assist the reader unfamiliar with LLNL abbreviations.